A Unified View of Some Numerical Methods for Fractional Diffusion

Clemens Hofreither

ÖAW RICAM

AANMPDE 12
Strobl, Austria
July 2019
1. The discrete eigenfunction method
2. Rational approximation methods
3. The BURA method
4. Rational approximations based on quadrature
5. The extension method
6. Time stepping method of Vabishchevich
7. Numerical study
1. The discrete eigenfunction method
2. Rational approximation methods
3. The BURA method
4. Rational approximations based on quadrature
5. The extension method
6. Time stepping method of Vabishchevich
7. Numerical study
Model problem

With $\Omega \subset \mathbb{R}^d$ a domain, $s \in (0, 1)$:

$$\mathcal{L}^s u = f \quad \text{in } \Omega,$$

$$u = 0 \quad \text{on } \partial \Omega,$$

where $\mathcal{L} u = -\text{div}(A \nabla u)$ s.p.d. diffusion operator.
Model problem

With $\Omega \subset \mathbb{R}^d$ a domain, $s \in (0, 1)$:

$$\mathcal{L}^s u = f \quad \text{in } \Omega,$$

$$u = 0 \quad \text{on } \partial \Omega,$$

where $\mathcal{L}u = -\text{div}(A\nabla u)$ s.p.d. diffusion operator.

**Use spectral definition:** for $u \in H^1_0(\Omega)$:

$$\mathcal{L}^s u = \sum_k \lambda_k^s(u, \varphi_k)\varphi_k$$

Nonlocal problem!
The discrete eigenfunction method (DEM)


- Galerkin discretization on $V_h \subset H^1_0(\Omega)$
- discrete eigensystem: $\mathcal{L}_hu_j^h = \lambda_j^hu_j^h, \ j = 1, \ldots, n$

\[
\mathcal{L}^s u \approx \sum_{j=1}^{n} (\lambda_j^h)^s (u, u_j^h) u_j^h
\]

\[
u_{DEM} := \sum_{j=1}^{n} (\lambda_j^h)^{-s} (f, u_j^h) u_j^h
\]
DEM in linear algebra terms

With stiffness/mass matrix $K, M \in \mathbb{R}^{n \times n}$: solve eigenproblem

$$Ku_j = \lambda_j^h Mu_j, \quad j = 1, \ldots, n,$$

where

- $\Lambda = \text{diag}(\lambda_j^h)_{j=1}^n$ matrix of eigenvalues,
- $U \in \mathbb{R}^{n \times n}$ matrix of eigenvectors.
DEM in linear algebra terms

With stiffness/mass matrix $K, M \in \mathbb{R}^{n \times n}$: solve eigenproblem

$$Ku_j = \lambda_j^h Mu_j, \quad j = 1, \ldots, n,$$

where

- $\Lambda = \text{diag}(\lambda_j^h)_{j=1}^n$ matrix of eigenvalues,
- $U \in \mathbb{R}^{n \times n}$ matrix of eigenvectors.

Let $f \in \mathbb{R}^n$ coefficient vector of $Q_h f \in V_h$.

$$u_{DEM} = U \Lambda^{-s} U^T M f = (M^{-1} K)^{-s} f.$$
DEM has quasi-optimal error

Using P1 FEM on a quasi-uniform mesh and under standard elliptic regularity assumptions, we have

$$\| u_{\text{exact}} - u_{\text{DEM}} \|_{L^2(\Omega)} \leq C \log(h^{-1}) h^{2s+2\delta} \| f \|_{H^{2\delta}}$$

for $f \in H^{2\delta}$, $\delta \leq 1 - s$.

DEM is slow: $O(n^3)$ operations for eigendecomposition.
Outline

1. The discrete eigenfunction method
2. Rational approximation methods
3. The BURA method
4. Rational approximations based on quadrature
5. The extension method
6. Time stepping method of Vabishchevich
7. Numerical study
Rational approximation methods

Assume we have a rational function \( r(z) \) such that

\[
    r(z) \approx z^{-s}
\]

We define

\[
    u_r = r(M^{-1}K)f.
\]

Theorem

Let \( u_r \in V_h \) from rational approximation. Then

\[
    \| u_{DE} - u_r \|_{L^2(\Omega)} \leq \max_{z \in [\lambda_{min}, \lambda_{max}]} |z - s - r(z)| \| f \|_{L^2(\Omega)}.
\]

(cf. [Harizanov et al., 2018] for a similar result)
Rational approximation methods

Assume we have a rational function $r(z)$ such that

$$r(z) \approx z^{-s}$$

We define

$$u_r = r(M^{-1}K)f.$$  

**Theorem**

Let $u_r \in V_h$ from rational approximation. Then

$$\|u_{DEM} - u_r\|_{L^2(\Omega)} \leq \max_{z \in [\lambda_{\min}, \lambda_{\max}]} |z^{-s} - r(z)| \|f\|_{L^2(\Omega)}.$$

(cf. [Harizanov et al., 2018] for a similar result)
Realizing a rational approximation method

If \( r \) is given in \textbf{partial fraction decomposition} form

\[
    r(z) = c_0 + \sum_{j=1}^{k} \frac{c_j}{z - d_j}, \quad c_j, d_j \in \mathbb{R},
\]

we obtain

\[
    u_r = r(M^{-1} K)f = c_0 + \sum_{j=1}^{k} c_j(M^{-1} K - d_j I_n)^{-1} f.
\]
Realizing a rational approximation method

If $r$ is given in **partial fraction decomposition** form

$$r(z) = c_0 + \sum_{j=1}^{k} \frac{c_j}{z - d_j}, \quad c_j, d_j \in \mathbb{R},$$

we obtain

$$u_r = r(M^{-1}K)f = c_0 + \sum_{j=1}^{k} c_j(M^{-1}K - d_jI)^{-1}f.$$  

With the solutions $w_j$ of

$$(K - d_jM)w_j = Mf, \quad j = 1, \ldots, k$$

(shifted diffusion problems), we can write

$$u_r = c_0 + \sum_{j=1}^{k} c_jw_j.$$  

If $d_j \leq 0$, then usually $K \approx K - d_jM$. **Nonpositive poles!**

→ **parallel realization**
1 The discrete eigenfunction method
2 Rational approximation methods
3 The BURA method
4 Rational approximations based on quadrature
5 The extension method
6 Time stepping method of Vabishchevich
7 Numerical study
Idea:

- compute BURA \( r(z) \) to \( z^{1-s} \) in \([0, 1]\) with degrees \((p, p)\)
- use \( \frac{r(z)}{z} \approx z^{-s} \) in \([0, 1]\)
- rescale original matrix such that \( \lambda_{\text{max}} \leq 1 \)
- \( \frac{r(z)}{z} \) has degrees \((p, p+1)\), PFD:

\[
\frac{r(z)}{z} = \sum_{j=1}^{p+1} \frac{c_j}{z - d_j}.
\]
Remarks on the BURA method

- $|r(z) - z^{1-s}|$ equioscillates, but

$$|r(z)/z - z^{-s}| = \frac{1}{z} |r(z) - z^{1-s}|$$

is large for small $z$

- using estimates from [Harizanov et al., 2018]:

$$\|u_{\text{DEM}} - u_{\text{BURA}}\|_{L^2(\Omega)} \lesssim \kappa^{1-s} E_{s,p} \|f\|_{L^2(\Omega)}$$

where $E_{s,p} \sim \exp(-\sqrt{(1-s)p})$

- improved approach: $\kappa$ eliminated

- computing BURAs is difficult
  - modified Remez algorithm
    - hard to implement
    - numerically unstable
  - even with quadruple precision, only $p \lesssim 11$ feasible
Rational approximations based on quadrature

Based on

\[ z^{-s} = \frac{2 \sin(\pi s)}{\pi} \int_{-\infty}^{\infty} \frac{e^{2sy}}{1 + e^{2y}z} \, dy, \]

three classes of quadrature rules are proposed. Third one:

\[ r_{BP3}(z) := \frac{2q \sin(\pi s)}{\pi} \sum_{\ell=-M}^{N} \frac{e^{2sy\ell}}{1 + e^{2y\ell}z}. \]

With proper parameter choices, they show:

\[ \max_z |z^{-s} - r_{BP3}(z)| \lesssim \exp(-\sqrt{p}) \]

where \( p \) is the degree of \( r_{BP3}(z) \).
1. The discrete eigenfunction method

2. Rational approximation methods

3. The BURA method

4. Rational approximations based on quadrature

5. The extension method

6. Time stepping method of Vabishchevich

7. Numerical study
Fractional Laplace as a Dirichlet-to-Neumann map

Idea

\((-\Delta)^s u\) in \(\Omega\) is the Neumann data of a local elliptic problem in \(\Omega \times (0, \infty)\) with Dirichlet data \(u\).

- Caffarelli, Silvestre 2007
- Stinga, Torrea 2010
- Capella, Dávila, Dupaigne, Sire 2011
- Brändle, Colorado, de Pablo, Sánchez 2013
- Nochetto, Otárola, Salgado 2015
Let $\alpha = 1 - 2s \in (-1, 1)$.

Find $U(x, y), x \in \Omega, y \in (0, \infty)$ such that

$$-\text{div}(y^\alpha \nabla U) = 0 \quad \text{in } \Omega \times (0, \infty),$$

$$\lim_{y \to \infty} U(x, y) = 0 \quad \forall x \in \Omega,$$

$$U(x, y) = 0 \quad \forall x \in \partial \Omega, y \in (0, \infty),$$

$$-(\lim_{y \to 0} y^\alpha \partial_y U(x, y)) = d_s f(x) \quad \forall x \in \Omega.$$

Then the solution is the Dirichlet trace

$$u(x) = (L^{-s}f)(x) = U(x, 0).$$
Numerical approach

- variational formulation in weighted Sobolev spaces
- can truncate extended direction (exponential convergence)
- discretization using tensor product spaces
- error analysis using P1-functions in $y$ direction

Numerical approach


- variational formulation in weighted Sobolev spaces
- can truncate extended direction (exponential convergence)
- discretization using tensor product spaces
- error analysis using P1-functions in $y$ direction

Higher-order discretizations in $y$ direction:
- Ainsworth, Glusa 2018
- Meidner, Pfefferer, Schürholz, Vexler 2018
- Banjai, Melenk, Nochetto, Otárola, Salgado, Schwab 2018
Discretization

Discretize using tensor product space built from:

- $V_h \subset H^1_0(\Omega)$ \hspace{1cm} $\dim V_h = n$
- $W_h$ FE space over $(0, Y)$, $w_h(Y) = 0$ \hspace{1cm} $\dim W_h = m$
Discretization

Discretize using tensor product space built from:

- \( V_h \subset H^1_0(\Omega) \) \( \dim V_h = n \)
- \( W_h \) FE space over \((0, Y), w_h(Y) = 0 \) \( \dim W_h = m \)

Can write stiffness matrix as:

\[
\mathcal{A}(\alpha) = M_y^{(\alpha)} \otimes K + K_y^{(\alpha)} \otimes M,
\]

where

- \( K, M \in \mathbb{R}^{n \times n} \) standard stiffness/mass matrices in \( V_h \)
- \( K_y^{(\alpha)}, M_y^{(\alpha)} \in \mathbb{R}^{m \times m} \) weighted stiffness/mass matrices in \( W_h \):

\[
[M_y^{(\alpha)}]_{ij} = \int_0^Y y^{\alpha} \psi_j(y) \psi_i(y) \, dy
\]

\[
[K_y^{(\alpha)}]_{ij} = \int_0^Y y^{\alpha} \psi'_j(y) \psi'_i(y) \, dy
\]
Theorem (H. 2019)

The solution of the discrete extended problem has the coefficient vector

\[ u_{EXM} = UEU^T Mf \]

with

\[ E = (e_1^T V \otimes I_n) D^{-1} (V^T e_1 \otimes I_n) \in \mathbb{R}^{n \times n} \]

Proof: based on a diagonalization argument and linear algebra.
Closed formula for the solution

**Theorem (H. 2019)**

The solution of the discrete extended problem has the coefficient vector

$$u_{EXM} = UEU^TMf$$

with

$$E = (e_1^TV \otimes I_n)D^{-1}(V^Te_1 \otimes I_n) \in \mathbb{R}^{n \times n}$$

*Proof*: based on a diagonalization argument and linear algebra.

Recall the Discrete Eigenfunction Method:

$$u_{DEM} = U\Lambda^{-s}U^TMf.$$

$$E \sim \Lambda^{-s}?$$
Doing some linear algebra, we find that $E$ is diagonal and

$$E = r(\Lambda), \quad r(z) = \sum_{k=1}^{m} \frac{v_k^h(0)^2}{\mu_k^h + z}.$$ 

where

- $\mu_k^h, k = 1, \ldots, m$ are discrete eigenvalues of the $y$ problem (1D),
- $v_k^h(y), k = 1, \ldots, m$ are discrete eigenfunctions of the $y$ problem (1D).
Connection to rational approximation

\[ u_{\text{DEM}} = U^s U^T Mf = (M^{-1} K)^{-s} f \]
\[ u_{\text{EXM}} = Ur(\Lambda) U^T Mf = r(M^{-1} K)f \]

with

\[ r(z) = \sum_{k=1}^{m} \frac{v_k^h(0)^2}{\mu_k^h + z}. \]

Extension method can be interpreted (realized, analyzed) as a rational approximation method!
Connection to rational approximation

\[ u_{DEM} = U^{\Lambda -s} U^T M f = (M^{-1} K)^{-s} f \]
\[ u_{EXM} = U r(\Lambda) U^T M f = r(M^{-1} K) f \]

with

\[ r(z) = \sum_{k=1}^{m} \frac{v_k^h(0)^2}{\mu_k^h + z}. \]

Extension method can be interpreted (realized, analyzed) as a rational approximation method!

\[ r(z) \approx z^{-s} \]
Relation to 1D Neumann-to-Dirichlet map

For $z > 0$, the discrete Galerkin solution $v \in W_h$ of the ODE

$$-(y^\alpha v'(y))' + z y^\alpha v(y) = 0 \quad \forall y \in (0, Y),$$

$$- \lim_{y \to 0^+} (y^\alpha v'(y)) = 1,$$

$$v(Y) = 0.$$

satisfies

$$r(z) = v(0).$$
Abstract error estimate for extension method

By studying the exact solution of the ODE and a duality-based error estimate, we can prove:

**Theorem (H. 2019)**

We have

$$\|u_{DEM} - u_{EXM}\|_{L^2(\Omega)} \leq E_{EXM}\|f\|_{L^2(\Omega)}$$

with

$$E_{EXM} = C_s \left( \exp( -2 \sqrt{\lambda_{\min}^h Y} ) \frac{\sqrt{\lambda_{\min}^h Y}}{\sqrt{\lambda_{\min}^h Y}} + \sup_{z \in [\lambda_{\min}^h, \lambda_{\max}^h]} \inf_{w_h \in W_h} \|v_z - w_h\|^2_b \right).$$
Abstract error estimate for extension method

By studying the exact solution of the ODE and a duality-based error estimate, we can prove:

**Theorem (H. 2019)**

We have

\[
\|u_{DEM} - u_{EXM}\|_{L^2(\Omega)} \leq E_{EXM} \|f\|_{L^2(\Omega)}
\]

with

\[
E_{EXM} = C_s \left( \exp\left(-2\sqrt{\frac{\lambda_{h \min} Y}{\lambda_{h \min}}}\right) + \sup_{z \in [\lambda_{h \min}, \lambda_{h \max}]} \inf_{w_h \in W_h} \|v_z - w_h\|_b^2 \right).
\]

**Ex:** for \(s = 1/2\) and using maximally smooth splines of degree \(p\) in \(y\)-direction, we obtain the rate \(O(m^{-2p})\).
Choose $\delta > 0$ such that $\mathcal{L} \geq \delta I$.

Find $w(t), t \in (0, 1)$ from the parabolic equation

$$(t(\mathcal{L} - \delta I) + \delta I) \frac{dw}{dt} + s(\mathcal{L} - \delta I)w = 0 \quad \forall t \in (0, 1), \quad w(0) = \delta^{-s}f.$$ 

Then the solution of the fractional diffusion problem is

$w(1)$. 

P.N. Vabishchevich. “Numerically solving an equation for fractional powers of elliptic operators.” J Comp Phys. 2015
Choose $\delta > 0$ such that $\mathcal{L} \geq \delta I$.

Find $w(t), t \in (0, 1)$ from the parabolic equation

$$(t(\mathcal{L} - \delta I) + \delta I) \frac{dw}{dt} + s(\mathcal{L} - \delta I)w = 0 \quad \forall t \in (0, 1), \quad w(0) = \delta^{-s} f.$$ 

Then the solution of the fractional diffusion problem is $w(1)$.

**Scalar equivalent:**

$$(t(z - \delta) + \delta)w'(t) + s(z - \delta)w(t) = 0$$

with the solution

$$w(t) = ((1 - t)\delta + tz)^{-s},$$

$$w(0) = \delta^{-s}, \quad w(1) = z^{-s}.$$
Discretization

Semidiscretization in space, $D := K - \delta M$:

$$(tD + \delta M)w' + sDw = 0 \quad \forall t \in (0, 1), \quad w(0) = \delta^{-s}f,$$

where $w : [0, 1] \rightarrow \mathbb{R}^n$. 
Discretization

Semidiscretization in space, \( D := K - \delta M \):

\[
(tD + \delta M)w' + sDw = 0 \quad \forall t \in (0, 1), \quad w(0) = \delta^{-s}f,
\]

where \( w : [0, 1] \rightarrow \mathbb{R}^n \).

**Time stepping:** Choose \( \theta \in (0, 1] \). For \( k \in \{0, \ldots, m\} \), denote

\[
t^k = \tau k, \quad \tau = \frac{1}{m},
\]

\[
t^{\theta(k)} := \theta t^{k+1} + (1 - \theta)t^k,
\]

\[
w^{\theta(k)} := \theta w^{k+1} + (1 - \theta)w^k
\]

and introduce the implicit scheme

\[
(t^{\theta(k)}D + \delta M)\frac{w^{k+1} - w^k}{\tau} + sDw^{\theta(k)} = 0 \quad \forall k = 0, \ldots, m - 1.
\]
Relation to rational approximation

**Theorem (H. 2019)**

The solution obtained by time stepping is given by

$$ u = Ur(\Lambda)U^{-1}f = r(M^{-1}K)f $$

with the rational function

$$ r(z) = \delta^{-s} \prod_{k=0}^{m-1} \omega_k(z), $$

$$ \omega_k(z) = \frac{\left( \frac{t^{\theta(k)}}{\tau} - s(1 - \theta) \right) (z - \delta) + \frac{\delta}{\tau}}{\left( \frac{t^{\theta(k)}}{\tau} + s\theta \right) (z - \delta) + \frac{\delta}{\tau}}, \quad k = 0, \ldots, m-1, $$

with degrees \((m, m)\). \(r(\cdot)\) has **nonpositive roots** if \(\theta = 0.5\).
Relation to rational approximation

Theorem (H. 2019)

The solution obtained by time stepping is given by

$$u = Ur(\Lambda)U^{-1}f = r(M^{-1}K)f$$

with the rational function

$$r(z) = \delta^{-s} \prod_{k=0}^{m-1} \omega_k(z),$$

$$\omega_k(z) = \frac{\left(\frac{t^{\theta(k)}}{\tau} - s(1 - \theta)\right)(z - \delta) + \frac{\delta}{\tau}}{\left(\frac{t^{\theta(k)}}{\tau} + s\theta\right)(z - \delta) + \frac{\delta}{\tau}}, \quad k = 0, \ldots, m - 1,$$

with degrees \((m, m)\). \(r(\cdot)\) has nonpositive roots if \(\theta = 0.5\).

This time stepping scheme can be interpreted as a rational approximation method – parallel realization!
1. The discrete eigenfunction method
2. Rational approximation methods
3. The BURA method
4. Rational approximations based on quadrature
5. The extension method
6. Time stepping method of Vabishchevich
7. Numerical study
Example

\[- \left( \frac{d^2}{dx^2} \right)^s u(x) = 1 \quad \forall x \in (-1, 1),\]
\[u(-1) = u(1) = 0\]

Linear FEM with 1024 elements.
eigenvalues of \(M^{-1}K\): \(\lambda^h_{\text{min}} \approx 9.87\), \(\lambda^h_{\text{max}} \approx 1.26 \cdot 10^7\).

All methods realized as rational approximation methods.
**Note:** convergence theorem is dimension independent.

We consider the spectral error

\[
\max_{z \in [\lambda_{\text{min}}, \lambda_{\text{max}}]} |z^{-s} - r(z)|
\]

and the \(L_2\)-error

\[
\| u_{\text{exact}} - u_r \|_{L_2(\Omega)}
\]
in dependence of the degree of the rational function \(r\).
Spectral error \( s = 0.5 \)
$L_2$ error – $s = 0.5$
Spectral error – \( s = 0.25 \)
$L_2$ error \(- s = 0.25\)
Spectral error – $s = 0.75$

![Graph showing spectral error over number of terms for different methods like BP3, BURA, EXM, EXM(3), AAA, Vab, and best. The y-axis represents the maximum error over the spectrum on a logarithmic scale, while the x-axis represents the number of terms also on a logarithmic scale. The graph illustrates the decrease in error as the number of terms increases.]
$L_2$ error – $s = 0.75$
The AAA method

Apply a black-box rational approximation method to

$$z^{-s}, \quad z \in [\lambda_{\text{min}}, \lambda_{\text{max}}].$$

Here:


Use the resulting rational function $r(z)$ for a rational approximation method.
Conclusion

- All presented methods can be interpreted and realized as rational approximation methods.
- The max-error of the rational approximation predicts the actual error in the $L_2$ norm well.
- The realization as a rational approximation method is inherently parallel.
- Better ways to get best rational approximations to $z^{-s}$?
  - Analytically – Zolotarev theory?
  - Numerically – continuation methods?

Code:
https://people.ricam.oeaw.ac.at/c.hofreither/